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Applications of Automatic Differentiation in Computational Fluid Dynamics

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Automatic differentiation (AD) is a powerful computational method that provides a means for computing exact sensitivity derivatives (SD) from existing computer programs for use in multidisciplinary design optimization (MDO) or in sensitivity analysis. The Mathematics and Computer Sciences Division of Argonne National Laboratory and the Center for Research on Parallel Computation at Rice University have developed a pre-compiler AD tool for FORTRAN programs called ADIFOR. The ADIFOR tool has been easily and quickly applied by NASA Langley researchers to assess the feasibility and computational impact of AD in MDO with several different FORTRAN programs. These include a state-of-the-art three-dimensional multigrid Navier-Stokes flow solver for wings or aircraft configurations in transonic turbulent flow. With ADIFOR, the user specifies sets of independent and dependent variables within an existing computer code. ADIFOR then traces the dependency path throughout the code, applies the chain rule to formulate derivative expressions, and generates new code to compute the required SD matrix. The resulting ADIFOR-generated codes have been verified to compute exact nongeometric and geometric SD, for a variety of cases, in less time than is required to compute the SD matrix using centered divided differences.

APPLICATIONS OF AUTOMATIC DIFFERENTIATION IN COMPUTATIONAL FLUID DYNAMICS

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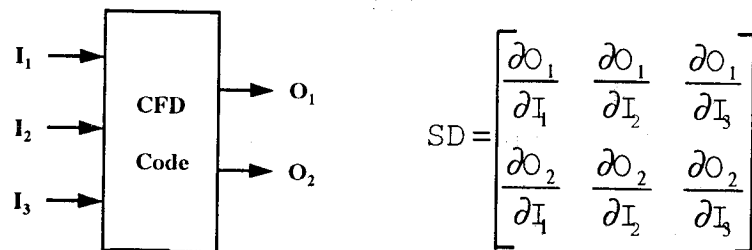
What are Sensitivity Derivatives?

- ◆ Sensitivity Derivatives (SD) describe how one thing changes with respect to another thing
- ◆ Example:
 - How a car's speed changes when braking
 - slowly at first, then more quickly
(how much)
 - speed decreases as braking increases
(which way)
- ◆ SD's describe how much and which way to change the variables in a multidisciplinary design optimization (MDO)

Objectives

- ◆ Obtain exact SD using the computational technique of Automatic Differentiation (AD)
- ◆ Assess the feasibility and computational impact of AD in a typical MDO problem

The SD Matrix



- ◆ Sample inputs: Mach number or geometry
- ◆ Sample outputs: wing pressure coefficients or grid
- ◆ SD matrix required in MDO

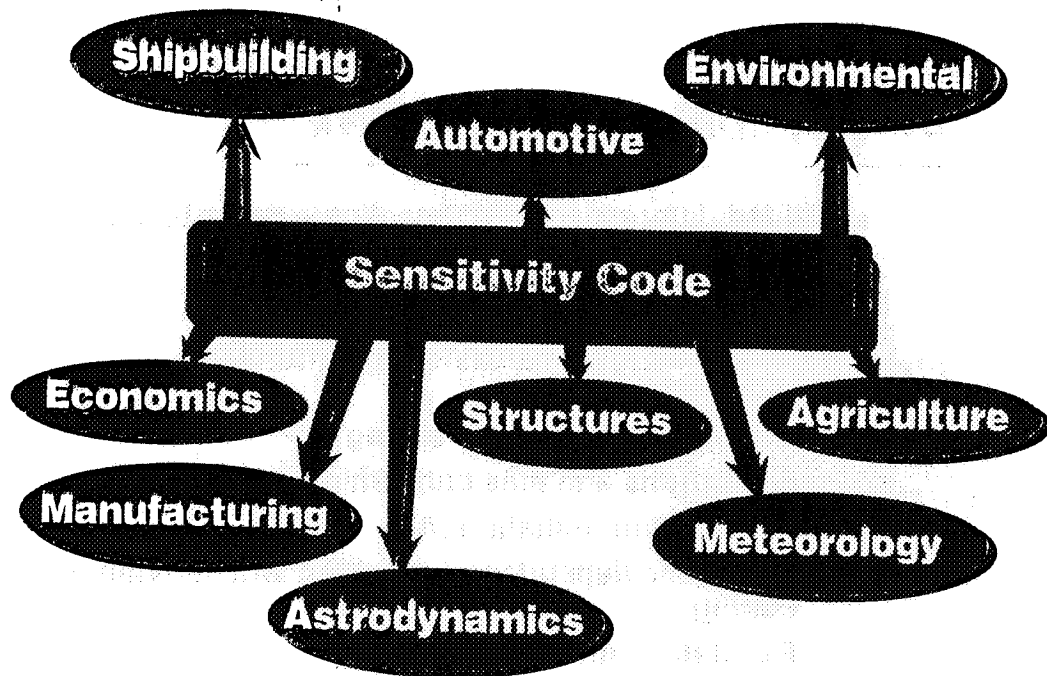
Calculation of the SD Matrix

- ◆ Divided differences (DD) (baseline + perturbations)
 - Proper step size difficult to determine
 - Truncation & resolution errors
- ◆ Hand coding (quasi-analytical) / symbolic manipulators
 - Manual dependency checking
 - Error prone and time consuming
- ◆ Automatic Differentiation (AD)
 - Automatic dependency checking and derivative coding
 - Exact derivatives via chain rule
 - Quick & easy; possible speed-up over DD

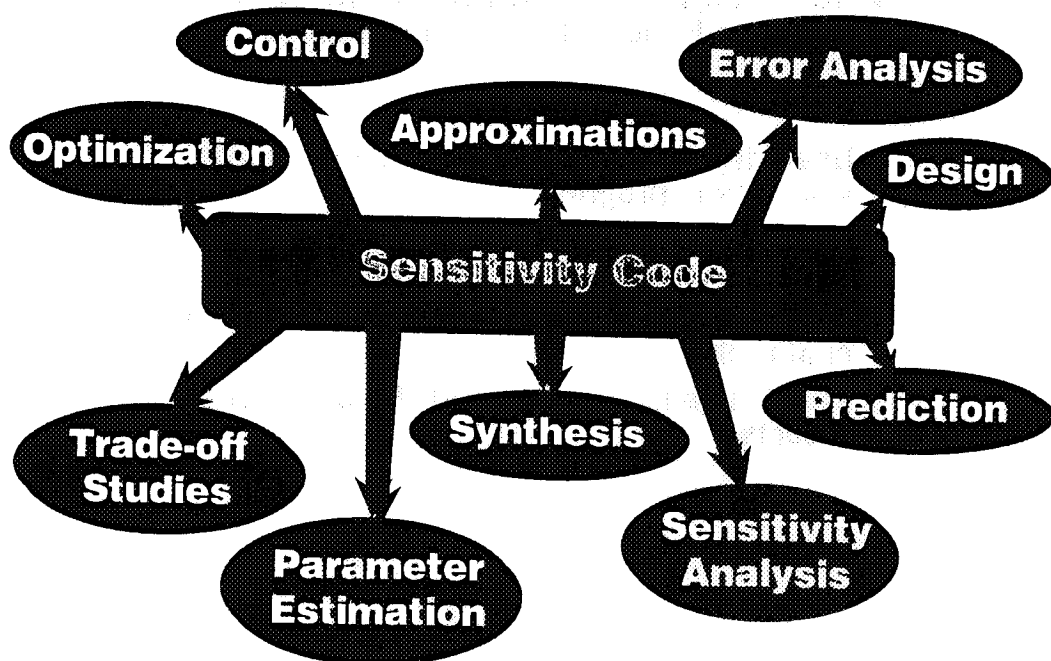
The AD Tool

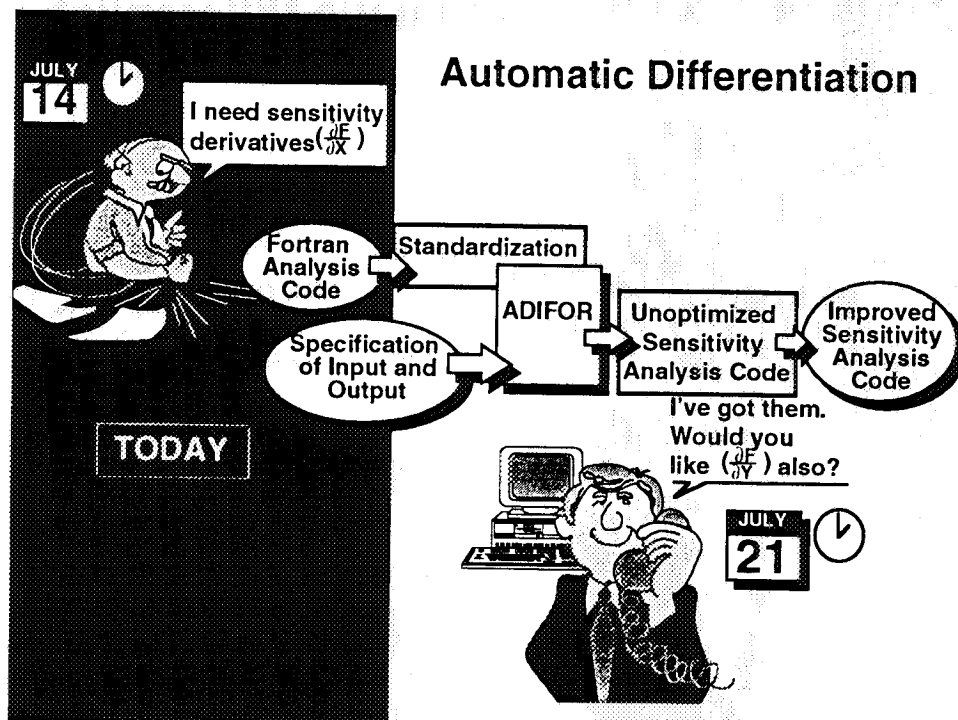
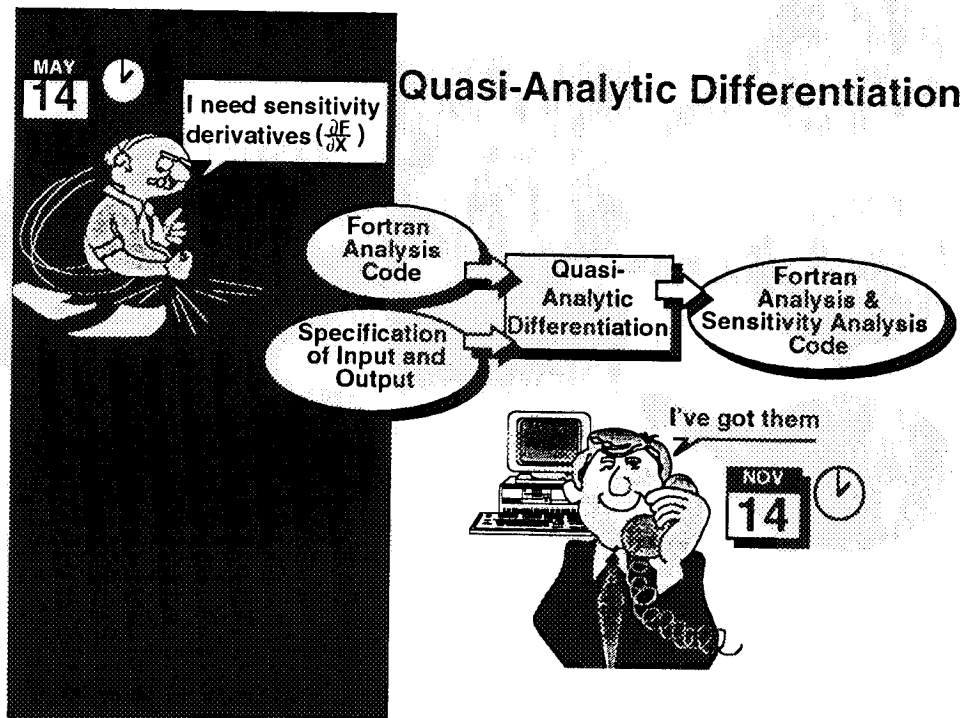
- ◆ ADIFOR (AD of FORTRAN) / PARASCOPE (Argonne National Laboratory and Rice University)
- ◆ User identifies dependent and independent variables in program
- ◆ ADIFOR follows program flow, traces program dependency paths
- ◆ ADIFOR formulates exact derivatives via the chain rule
- ◆ ADIFOR generates new code for derivative objects

Potential ADIFOR Use: By Application

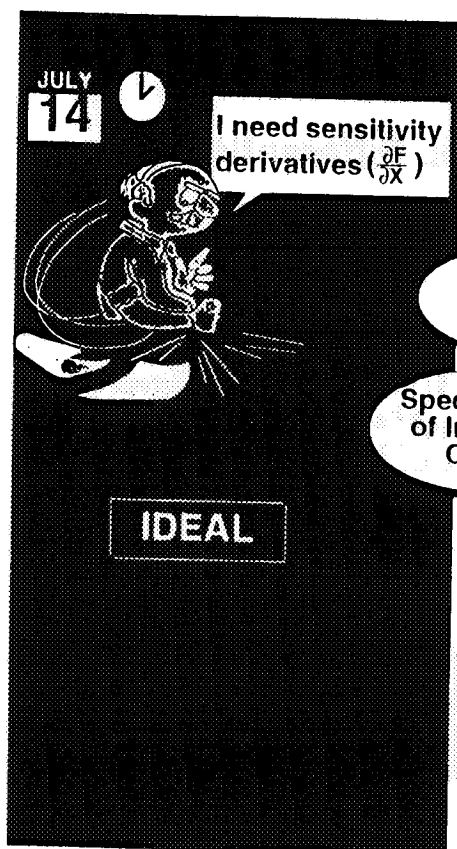
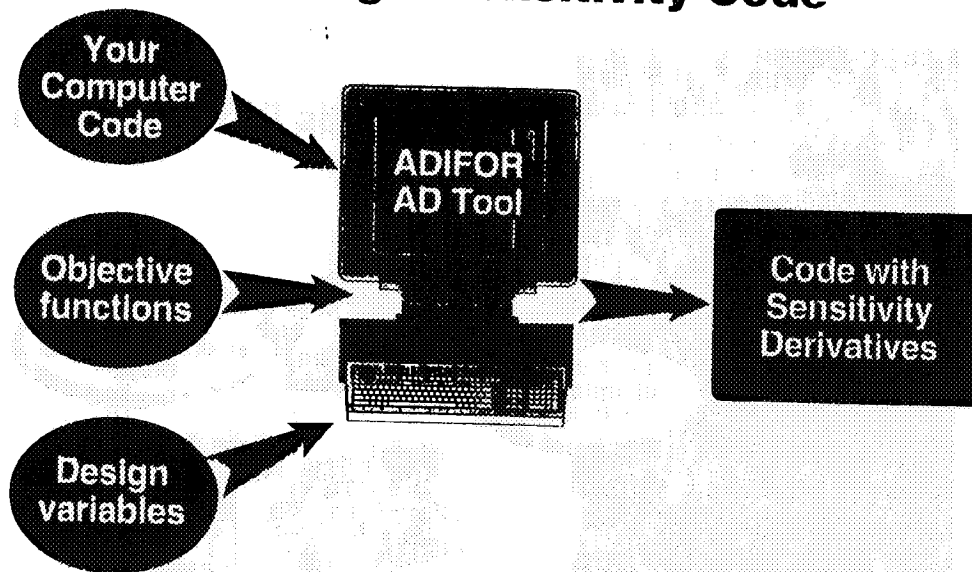


Potential ADIFOR Use: By Problem Type

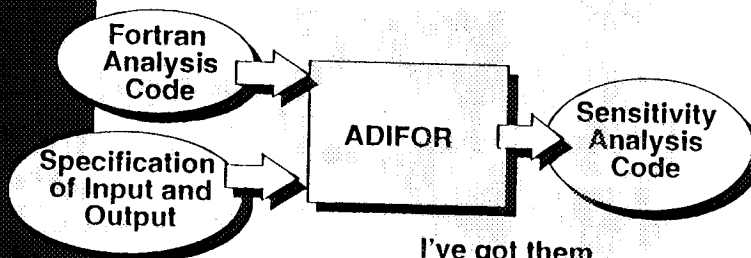




Building a Sensitivity Code



Automatic Differentiation



The CFD Codes

- ◆ WTCO: wing C-O grid generation
 - Algebraic
 - Transfinite interpolation
- ◆ TLNS3D: 3-D thin-layer Navier-Stokes solver
 - Finite-volume, central-differencing
 - Grid sequencing, multigrid
 - Scalar artificial dissipation
 - Baldwin-Lomax turbulence model

ADIFOR Applications in CFD

- ◆ WTCO wing grid generation program
 - Independents: thickness, c_{max} , twist
 - Dependents: grid coordinates (x, y, z)
- ◆ TLNS3D Navier-Stokes flow solver
 - Independents: grid coordinates (x, y, z)
 - Dependents: pressure coefficients (C_p)

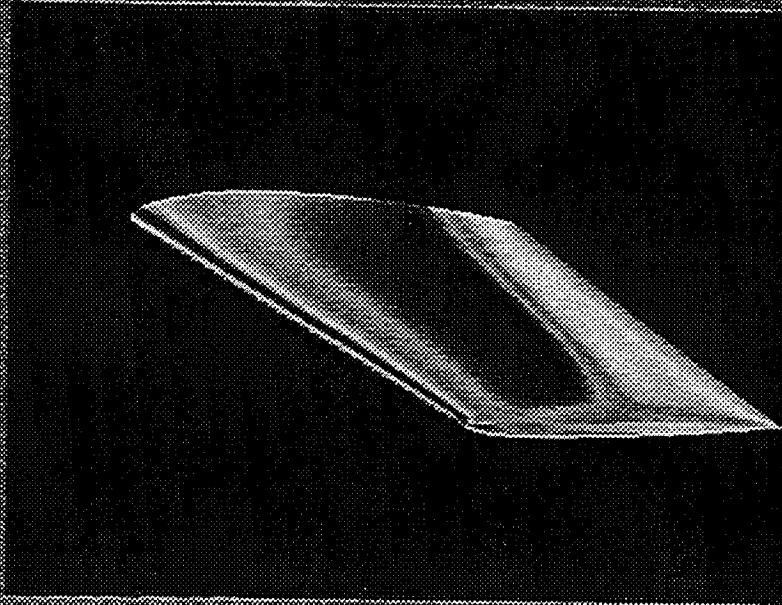
ADIFOR Applications in CFD

- ◆ WTCO wing grid generation program
 - Independents: thickness, cmax, twist
 - Dependents: grid coordinates (x, y, z)
- ◆ TLNS3D Navier-Stokes flow solver
 - Independents: grid coordinates (x, y, z)
 - Dependents: pressure coefficients (C_p)
- ◆ WTCO-TLNS3D coupling via file transfer
 - Grid
 - Grid SD matrix
 - Application of chain rule $\frac{\partial(Flow)}{\partial(Sect)} = \frac{\partial(Flow)}{\partial(Grid)} \frac{\partial(Grid)}{\partial(Sect)}$

Computational Results

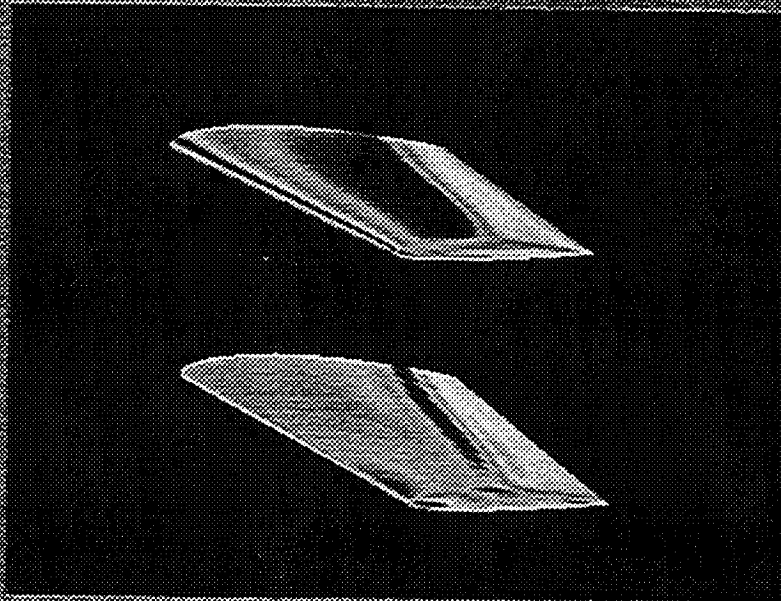
- ◆ ONERA M6 wing planform
- ◆ NACA 2412 airfoil sections
- ◆ $97 \times 25 \times 17$ grid
- ◆ $M_\infty = 0.84$, $\alpha = 0.00$, $Re = 11.7 \times 10^6$
- ◆ Wing C_p and SD of wing C_p
- ◆ Coloring: white/red = large, blue/black = small
- ◆ Several geometries:
 - baseline
 - thickness perturbations \pm
 - cmax perturbations \pm
 - twist perturbations \pm

Flow over a wing, $M=0.84$



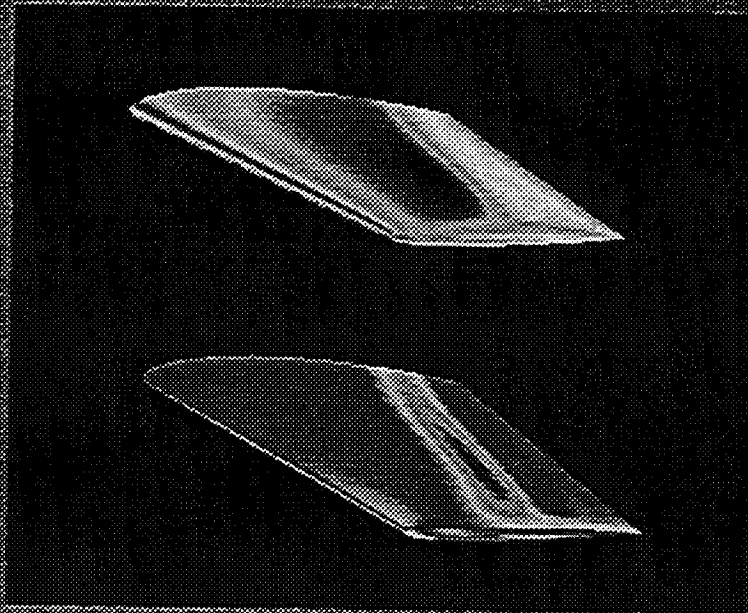
♦ Pressure coefficient (C_p)

SD for wing via AD, $M=0.84$



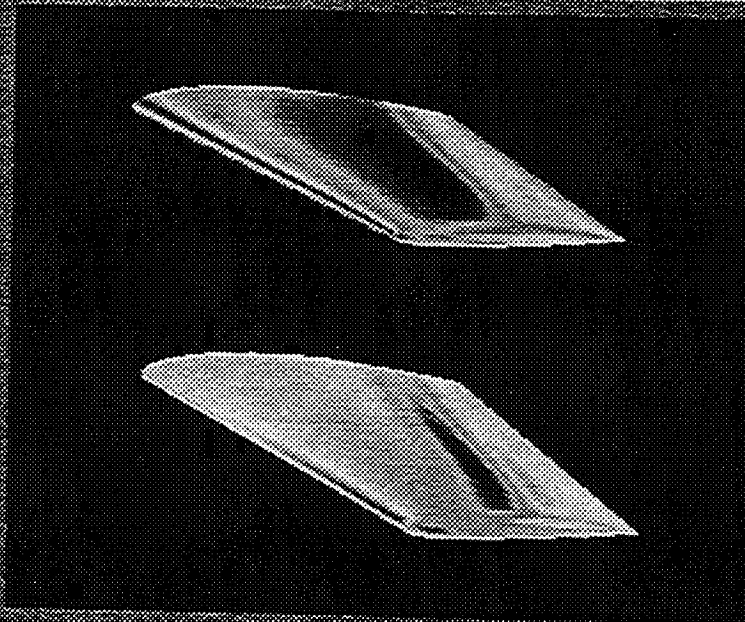
♦ C_p and $(dC_p/d\text{twist})$ for several geometries

SD for wing via AD, $M=0.84$



◆ C_p and $(dC_p/d\epsilon)_{\max}$ for several geometries

SD for wing via AD, $M=0.84$



◆ C_p and $(dC_p/d\epsilon)_{\max}$ for several geometries

Summary

- ♦ Feasibility of using AD in CFD demonstrated
- ♦ ADIFOR calculated exact geometric SD for grid-flow coupling similar to MDQ problem
- ♦ ADIFOR calculated SD through complex algorithm for nonlinear problem
- ♦ ADIFOR processing easier & faster than quasi-analytic method
- ♦ AD competitive with & more accurate than divided differences

Special thanks to...

- ♦ Veer Vatsa for use of TLNS3D code
- ♦ Mary Adams for FAST animation sequences
- ♦ Thomas Roberts for PowerBook movies
- ♦ John Knox for video production
- ♦ Thomas Zang for continued support
- ♦ Laura Hall, Andreas Griewank, and George Corliss for initial training and support with ADIFOR

**Sensitivity Derivatives =
BETTER**

**Multidisciplinary Design
Optimization =
PRODUCTS & PROCESSES**

**Automatic Differentiation =
EASILY, QUICKLY & RELIABLY**